

chain nodes :

13 14 19 20 21 22 23 31 33

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 27 28 29 30

chain bonds :

5-9 13-14 20-21 22-23 31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 11-27 12-30 27-28  
28-29 29-30

exact/norm bonds :

5-9 7-8 7-12 8-9 9-10 10-11 11-12 11-27 12-30 13-14 20-21 22-23 31-33

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 27-28 28-29 29-30

isolated ring systems :

containing 1 : 7 :

G1:CH2,O,[\*1]

G2:[\*2],[\*3],[\*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:CLASS 14:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 27:Atom  
28:Atom 29:Atom 30:Atom 31:CLASS 32:Atom 33:Atom

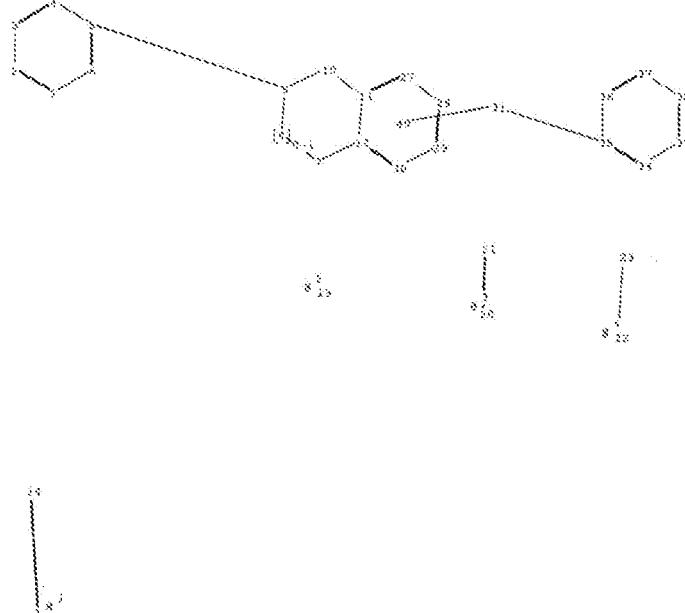
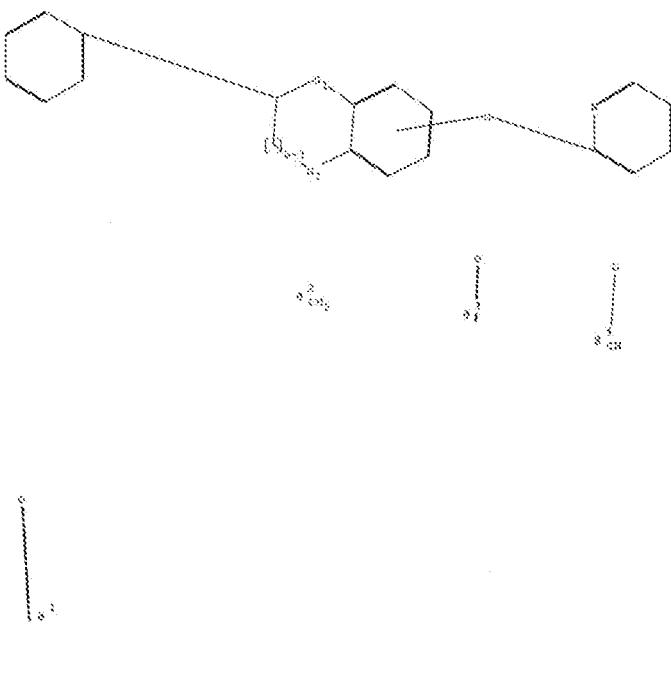
Generic attributes :

33:

Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Number of Hetero Atoms : Exactly 1  
Type of Ring System : Monocyclic

Element Count :

Node 33: Limited  
C, C5  
N, N1



chain nodes :

13 14 19 20 21 22 23 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 27 28 29 30 34 35 36 37 38 39

chain bonds :

5-9 13-14 20-21 22-23 31-35

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 11-27 12-30 27-28  
28-29 29-30 34-35 34-39 35-36 36-37 37-38 38-39

exact/norm bonds :

5-9 7-8 7-12 8-9 9-10 10-11 11-12 11-27 12-30 13-14 20-21 22-23 31-35

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 27-28 28-29 29-30 34-35 34-39 35-36 36-37 37-38  
38-39

isolated ring systems :

containing 1 : 7 :

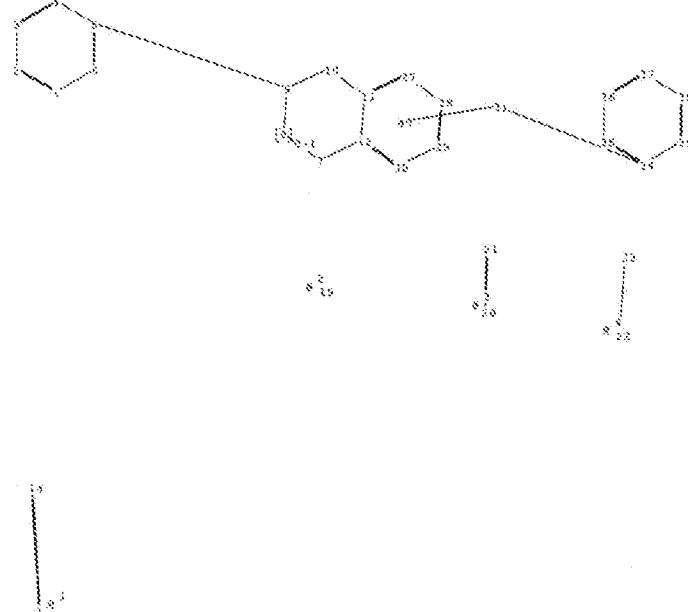
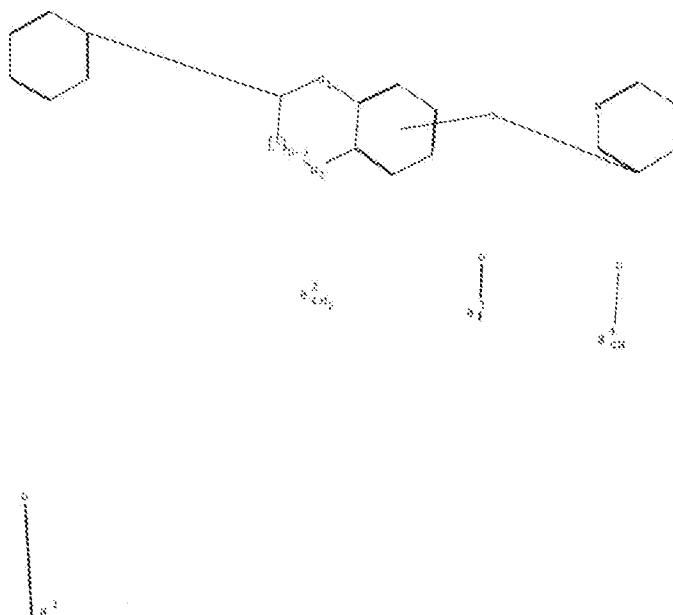
G1:CH2,O,[\*1]

G2:[\*2],[\*3],[\*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:CLASS 14:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 27:Atom  
28:Atom 29:Atom 30:Atom 31:CLASS 34:Atom 35:CLASS 36:CLASS 37:Atom 38:Atom  
39:Atom 40:Atom





chain nodes :

13 14 19 20 21 22 23 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 27 28 29 30 34 35 36 37 38 39

chain bonds :

5-9 13-14 20-21 22-23 31-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 11-27 12-30 27-28  
28-29 29-30 34-35 34-39 35-36 36-37 37-38 38-39

exact/norm bonds :

5-9 7-8 7-12 8-9 9-10 10-11 11-12 11-27 12-30 13-14 20-21 22-23 31-34

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 27-28 28-29 29-30 34-35 34-39 35-36 36-37 37-38  
38-39

isolated ring systems :

containing 1 : 7 :

G1:CH2,O, [\*1]

G2:[\*2], [\*3], [\*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:CLASS 14:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 27:Atom  
28:Atom 29:Atom 30:Atom 31:CLASS 34:Atom 35:CLASS 36:CLASS 37:Atom 38:Atom  
39:Atom 40:Atom

=> d his

(FILE 'HOME' ENTERED AT 18:12:05 ON 25 FEB 2008)

FILE 'REGISTRY' ENTERED AT 18:12:10 ON 25 FEB 2008

L1           STRUCTURE uploaded  
L2           0 S L1  
L3           STRUCTURE uploaded  
L4           0 S L3  
L5           STRUCTURE uploaded  
L6           1 S L5  
L7           218 S L5 FULL

FILE 'HCAPLUS' ENTERED AT 18:23:44 ON 25 FEB 2008

L8           2 S L7

FILE 'CAOLD' ENTERED AT 18:23:56 ON 25 FEB 2008

L9           0 S L7

FILE 'REGISTRY' ENTERED AT 18:24:05 ON 25 FEB 2008

L10          STRUCTURE uploaded  
L11          0 S L10  
L12          1 S L10 FULL

FILE 'HCAPLUS' ENTERED AT 18:25:12 ON 25 FEB 2008

L13          1 S L12

FILE 'CAOLD' ENTERED AT 18:25:24 ON 25 FEB 2008

L14          0 S L12

FILE 'REGISTRY' ENTERED AT 18:25:31 ON 25 FEB 2008

L15          STRUCTURE uploaded  
L16          0 S L15  
L17          1 S L15 FULL  
L18          1 S L17 NOT L12

FILE 'HCAPLUS' ENTERED AT 18:26:47 ON 25 FEB 2008

L19          1 S L18

FILE 'CAOLD' ENTERED AT 18:26:57 ON 25 FEB 2008

L20          0 S L18

FILE 'REGISTRY' ENTERED AT 18:27:04 ON 25 FEB 2008

L21          STRUCTURE uploaded  
L22          0 S L21  
L23          0 S L21 FULL  
L24          STRUCTURE uploaded  
L25          0 S L24  
L26          0 S L24 FULL  
L27          STRUCTURE uploaded  
L28          13 S L27  
L29          219 S L27 FULL  
L30          2 S L29 NOT L7

FILE 'HCAPLUS' ENTERED AT 18:32:18 ON 25 FEB 2008

L31          1 S L30

FILE 'CAOLD' ENTERED AT 18:32:27 ON 25 FEB 2008

L32          0 S L30

L33           'REGISTRY' ENTERED AT 18:32:34 ON 25 FEB 2008  
L34           STRUCTURE uploaded  
L35           0 S L33  
L35           1 S L33 FULL

L36           FILE 'HCAPLUS' ENTERED AT 18:33:46 ON 25 FEB 2008  
L36           1 S L35

L37           FILE 'CAOLD' ENTERED AT 18:33:56 ON 25 FEB 2008  
L37           0 S L35

L38           FILE 'REGISTRY' ENTERED AT 18:34:03 ON 25 FEB 2008  
L38           STRUCTURE uploaded  
L39           0 S L38  
L40           1 S L38 FULL  
L41           1 S L40 NOT L36

L42           FILE 'HCAPLUS' ENTERED AT 18:35:16 ON 25 FEB 2008  
L42           1 S L41

L43           FILE 'CAOLD' ENTERED AT 18:35:35 ON 25 FEB 2008  
L43           0 S L41

L44           FILE 'REGISTRY' ENTERED AT 18:35:42 ON 25 FEB 2008  
L44           STRUCTURE uploaded  
L45           1 S L44  
L46           STRUCTURE uploaded  
L47           1 S L46  
L48           220 S L46 FULL

L49           FILE 'HCAPLUS' ENTERED AT 18:39:17 ON 25 FEB 2008  
L49           2 S L48

L50           FILE 'CAOLD' ENTERED AT 18:39:48 ON 25 FEB 2008  
L50           0 S L48

L51           FILE 'REGISTRY' ENTERED AT 18:39:56 ON 25 FEB 2008  
L51           STRUCTURE uploaded  
L52           0 S L51  
L53           1 S L51 FULL  
L54           1 S L53 NOT L41

L55           FILE 'HCAPLUS' ENTERED AT 18:41:08 ON 25 FEB 2008  
L55           1 S L54

L56           FILE 'CAOLD' ENTERED AT 18:41:21 ON 25 FEB 2008  
L56           0 S L55

L57           FILE 'REGISTRY' ENTERED AT 18:41:29 ON 25 FEB 2008  
L57           STRUCTURE uploaded  
L58           0 S L57  
L59           1 S L57 FULL

L60           FILE 'HCAPLUS' ENTERED AT 18:42:41 ON 25 FEB 2008  
L60           1 S L59

L61           FILE 'CAOLD' ENTERED AT 18:42:50 ON 25 FEB 2008  
L61           0 S L59

L62           FILE 'REGISTRY' ENTERED AT 18:42:58 ON 25 FEB 2008  
L62           STRUCTURE uploaded

L63            3 S L62  
L64            451 S L62 FULL

FILE 'HCAPLUS' ENTERED AT 18:44:36 ON 25 FEB 2008  
L65            2 S L64  
L66            1 S L65 NOT L49  
L67            1 S L66 NOT L50

FILE 'CAOLD' ENTERED AT 18:45:39 ON 25 FEB 2008

=> S L64  
L68            O L64